

512a Atomic-Scale Analysis of Ductile Void Growth and Nanocrystalline Domain Formation as Strain Relaxation Mechanisms in Ultra-Thin Metallic Films

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Understanding the atomistic mechanisms of strain relaxation in ultra-thin metallic films is essential for improving the reliability of microelectronic devices and advancing nanofabrication techniques. Atomic-scale modeling based on molecular-dynamics (MD) simulations provides a powerful means for analyzing atomistic mechanisms of strain relaxation in metallic thin films and enables the development of constitutive relationships for continuum modeling of metallic thin-film mechanical behavior. The results of such modeling are particularly important for predictions of materials reliability in current and future electromechanical device technologies, where nano-scale features become increasingly important.

In this presentation, we report a comprehensive computational analysis of the atomistic mechanisms of strain relaxation over a wide range (up to 17%) of applied biaxial tensile strain in free-standing Cu thin films with the film plane oriented normal to the [111] crystallographic direction. The analysis is based on isothermal-isostrain MD simulations within an embedded-atom-method (EAM) parameterization for Cu and using slab supercells that contain millions of atoms. We have carried out simulations with and without cylindrical voids normal to the film plane and extending throughout the film thickness.

Our analysis has revealed various regimes in the film's mechanical response as the applied biaxial strain level increases. After an elastic response at low strain ($< 2\%$), plastic deformation occurs accompanied by dislocation emission from the void surface, void surface morphological transition, dislocation jogging, vacancy generation due to gliding of jogged dislocations, vacancy pipe diffusion along dislocation cores, dislocation-vacancy and dislocation-dislocation interactions, as well as formation and propagation of threading dislocation loops. Over the strain range following the elastic-to-plastic deformation transition ($< 8\%$), void growth is the major strain relaxation mechanism mediated by emission of perfect screw dislocations from the void surface and subsequent dislocation propagation; as a result, a plastic zone forms around the void and extends radially outwards over time. At higher levels of applied strain ($> 8\%$), a subsequent transition to a new strain relaxation regime gives rise to a practically uniform distribution of dislocations in the metallic thin film. Under such conditions, formation of nanometer-scale twinned domains of fcc crystalline material mediates the transformation of the initially single-crystalline metallic film to a nanocrystalline structure. Furthermore, void growth is inhibited as the dislocations emitted from the void surface are pinned by their interaction with the simultaneously generated network of defects in the nanocrystalline material. By comparing MD simulation results in identical thin films with and without voids, it is also demonstrated that strain relaxation at high levels of strain ($\geq 12\%$) is not affected by a pre-existing void in the metallic film.